# Second Moment Method for Evaluating Human Health Risks from Groundwater Contaminated by Trichloroethylene

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Pollutants in groundwater aquifers may constitute a significant human health risk. A large variation in response may result among human populations experiencing the same level and duration of exposure to pollutants. Variability in response, as a result of exposure to a carcinogenic contaminant such as trichloroethylene (TCE), can be represented by a distribution function of safe doses. Spatial variability in aquifer characteristics and contaminant transport parameters requires the use of stochastic transport models to quantify variability in exposure concentrations. A second moment method is used to evaluate the probability of exceeding safe dose levels for a contaminated aquifer. The name of this method stems from the fact that the formulation is based on the first and second moments of the random variables. With this method, the probability is a function of the variability of contaminant concentration (which incorporates variability in hydrogeologic parameters such as hydraulic conductivity) and the variability in response in the human population. In this manner, the severity of the health risk posed by a contaminated aquifer and the evaluation of appropriate strategies and technologies for aquifer remediation are a function of contaminant concentrations and human health risks. The applicability and limitations of this method are demonstrated with data on groundwater contaminated by TCE at Hill Air Force Base, Utah. *Key words*: contaminant transport, groundwater flow, health risk, second moment method, stochastic modeling, trichloroethylene. *Environ Health Perspect* 104:866–870 (1996)

Prioritizing the remediation of contaminated aquifers has very large economic and human health implications. When carcinogenic contaminants are present in groundwater, human health risks must be estimated because the water may be used for drinking, washing food, and bathing. Contaminants may enter groundwater as a result of burial or deep-well injection of hazardous wastes into the subsurface or migration into the subsurface from surface impoundments. Because remediation is usually a long-term and expensive process, it is important to develop methods to determine which contaminated aquifers pose the greatest health risks. In some cases, containment rather than remediation may be the most appropriate strategy. In this paper the term remediation includes all processes, technologies, and water management strategies that reduce contaminant concentrations in groundwater aquifers. In addition to setting priorities for remediation, it is important to estimate health risks to determine and evaluate the effectiveness of methods and technologies that are either available or are being considered to remediate contaminated aquifers. In this paper, the human health risk under consideration is the probability of cancer as a result of life-time exposure to trichloroethylene (TCE) in drinking water from groundwater aquifers. Using data on TCE concentrations measured in a contaminated aquifer, a method is described for estimating carcinogenic risks by incorporating the uncertainties associated with the groundwater flow and

solute transport process and the variability of safe dose levels for a diverse population.

TCE is a volatile, nonflammable chlorinated aliphatic hydrocarbon used extensively as a metal degreasing solvent. The International Agency for Research on Cancer (IARC) has listed TCE as a Group 3 carcinogen in humans (1). The classification is based on inadequate evidence of carcinogenicity in humans and limited evidence of carcinogenicity in experimental animal studies. A review of other acute and chronic toxic effects of TCE is detailed in a technical report by the Agency for Toxic Substances and Disease Registry (2).

In developing water quality standards for groundwater, the U.S. Environmental Protection Agency (EPA) uses ambient water quality standards that have been developed for surface waters such as lakes, streams, rivers, and ponds. For TCE, the EPA has established a life-time exposure standard of 5 μg/l (3) and the World Health Organization (WHO) has established a short-term exposure standard of 70 μg/l for exposures greater than 14 days but less than 12 months (4).

Methods for quantifying cancer risks as a result of lifetime low-level exposure to chemical carcinogens (5–7) calculate either a single or a narrow range of safe doses for a very low risk of cancer, usually one in a million. For individual members of a diverse human population, however, a wide range of outcomes is usually observed as a result of life-time exposure to carcinogenic

chemicals (8). A diverse human population includes males, females, children, and elderly individuals with different genetic characteristics and varying states of health. Support for including variability in safe doses comes from a study by Portier and Kaplan (9). In this study, variability in safe doses was obtained by defining the variables in a physiologically based pharmacokinetic (PBPK) model for methylene chloride in probabilistic terms. PBPK models describe physiological and metabolic functions and processes that affect the distribution of chemicals and their metabolites in different organs and tissues. An important component of the carcinogenic mechanism of methylene chloride is metabolic activation by glutathione S-transferase. In human populations, there exists considerable variability in the rate coefficients for the enzyme-mediated metabolism of methylene chloride, thereby resulting in varying biological concentrations of reactive metabolites in tissues and organs. In this study, it was shown that as the variance in metabolic rate parameters increased the mean or average safe dose remained about the same; however, the variance in safe exposure doses increased (9). These results suggest that safe doses in a diverse human population may be uncertain and are better represented probabilistically.

Groundwater contaminant concentrations at pumping well locations vary as a result of imposed hydraulic transients. Furthermore, natural groundwater systems are rarely uniform and homogeneous. For a particular contaminated aquifer, values of transport parameters such as hydraulic conductivity, dispersivity, and sorption coefficients to soil surfaces can vary significantly from location to location. Due to this subsurface heterogeneity, stochastic models are required to describe solute transport uncer-

tainty. For these models, parameters describing the transport process are represented by distribution functions with prescribed means and variances. Therefore, calculated contaminant concentrations at pumping wells are described probabilistically.

## Second Moment Formulation

The second moment formulation is commonly used by structural engineers to evaluate the probability of failure of structural elements such as beams under variable loading conditions (*10*). In the analysis of beam failure under variable loading conditions, probability distribution functions are required to describe the variability in beam load-carrying capacity and to describe the variability in beam loading. In this study, the second moment formulation is used to determine if the distribution of concentrations of TCE in a contaminated aquifer exceeds the distribution of safe doses in a diverse human population (*10–12*). In this manner, carcinogenic health risks posed by drinking groundwater from a contaminated pumping well can be estimated.

In this analysis, the concentration of a contaminant (*C*; e.g., TCE in µg/l) within the subsurface is modeled as a random variable with a known mean, variance, and distribution. Variable safe doses are also modeled as a random variable (*R*) with known mean, variance, and distribution. At any time, the safe dose level should be greater than the concentration of contaminant encountered. That is $R > C$. Similarly, if $R < C$, the contaminant concentration exceeds the safe dose. As a probability, this event is expressed as

$$P_f = P(R < C) \qquad (1)$$
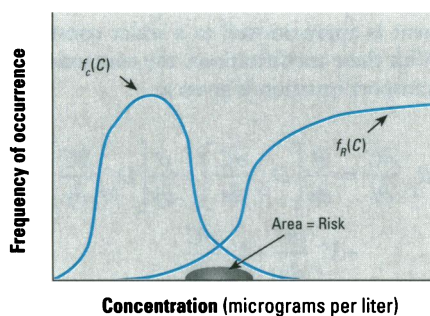


**Figure 1.** Graphical representation of the second moment method. $f_c(C)$ represents the distribution function of contaminant concentrations in groundwater from a pumping well located in the contaminant plume. $F_R(C)$ is the cumulative distribution function for safe doses for this contaminant for a diverse human population. The area of overlap of these two distribution functions is the probability that contaminant concentrations in groundwater exceed safe dose concentrations. This probability, $P_f$, is computed by the convolution integral of Equation 2.

where $P_f$ is defined as the probability that contaminant concentrations exceed the safe dose. The subscript of *f* indicates that this is a probability of failure, e.g., contaminant concentrations in groundwater exceed safe exposure doses. Letting $f_r(r)$ and $f_c(c)$ define the distribution of safe doses and the distribution of contaminant concentrations, respectively, the probability that contaminant concentrations exceed the safe dose is defined as

$$P_f = \int_0^\infty F_r(C) f_c(C) dC \qquad (2)$$

where $F_r(C)$ is the cumulative distribution function of $f_r(r)$ evaluated at *C*. Figure 1 illustrates Equation 2.

The method is simplified if the functions for $f_r(r)$ and $f_c(c)$ are normally distributed. In this case, the probability that contaminant concentrations exceed the safe dose can be stated in terms of the means, $\mu_r$ and $\mu_c$, and variances, $\sigma_r$ and $\sigma_c$, of the normally distributed random variables and takes advantage of the characteristics of the standard normal distribution. Using reduced variates of the standard normal distribution, a safety index ($\beta$) is derived. Geometrically, $\beta$ is defined as the shortest distance from the origin of the reduced variates to the limit state where the safe dose concentration is equal to the pollutant concentration. Mathematically, $\beta$ is defined as

$$\beta = \frac{\mu_r - \mu_c}{\sqrt{\sigma_r^2 + \sigma_c^2}} \qquad (3)$$

Using the safety index, the probability that contaminant concentrations will exceed the safe dose reduces to

$$P_f = 1 - \Phi\left[\frac{\mu_r - \mu_c}{\sqrt{\sigma_r^2 + \sigma_c^2}}\right] \qquad (4)$$

where $\Phi(\cdot)$ represents the standard normal distribution function.

The approach presented in Equations 1 through 4 is often called the second moment formulation (*10,11*). The name stems from the fact that the model requires only the distribution means and standard deviations that are functions of the first and second moments of the distributions. Equations 3 and 4 are useful only if both distributions are normally distributed or are assumed to be normally distributed. If the data are found to be other than normally distributed, an alternative solution strategy must be used. One method is to transform the true distribution into an equivalent normal distribution using the Rosenblatt transform (*10*). Alternatively,

the convolution integral of Equation 2 may be solved directly using any appropriate numerical integration technique.

## Aquifer and Contaminant Characteristics

The contaminated aquifer used in this study is designated as Operational Unit 3 (OU3) and is located at Hill Air Force Base (AFB) near Ogden, Utah (*8*). There are four hydrogeological components of the aquifer; however, simulations were only required for the one contaminated shallow water table aquifer directly beneath Hill AFB. The contaminated area of the shallow aquifer consists of 50% lacustrine clay and 50% lacustrine sands. The thickness of the shallow aquifer is between 100 to 200 feet. Hydraulic conductivities range from a low of $10^{-6}$ ft/day to a high of $10^2$ ft/day. The average storage coefficient is estimated to be 0.2 with a range of 0.01–0.3 and the average retardation factor for TCE is 11.8 with a range of 4.5–28. In this study, hydraulic conductivity is modeled as a spatially varying random variable. A plan view of Hill AFB is shown in Figure 2, showing the north–south orientation of the contaminant plume and primary direction of flow in the contaminated aquifer.

## Model Simulations

To illustrate the methodology presented in Equations 1 through 4 for evaluating the health risks of a contaminated aquifer, TCE transport behavior was analyzed with a two-dimensional (2-D) finite difference contaminant transport model based on the method of characteristics (MOC) (*12,13*). This model has been modified to run successive Monte Carlo simulations to account for subsurface heterogeneity (*12,14,15*). In the development of model transport equations, the units given in the definitions for variables and parameters in groundwater flow and contaminant transport equations have been written in the basic units of length (*L*), time (*t*) and mass (*M*). The model is composed of a coupled groundwater flow and contaminant transport model. The 2-D groundwater flow is given as

$$S_t \frac{\partial h}{\partial t} + W(x, y, t)$$
$$= \frac{\partial}{\partial x}\left[K_{xx} \frac{\partial h}{\partial x}\right] + \frac{\partial}{\partial y}\left[K_{yy} \frac{\partial h}{\partial y}\right] \qquad (5)$$

where $S_t$ is the storage coefficient or storativity of the aquifer (dimensionless), *h* is hydraulic head (*L*), $W(x,y,t)$ is the volume flux per unit area of the source term (positive for outflow and negative for inflow; $L\ t^{-1}$), and $K_{xx}$ and $K_{yy}$ are the *xx*- and *yy*-diagonal
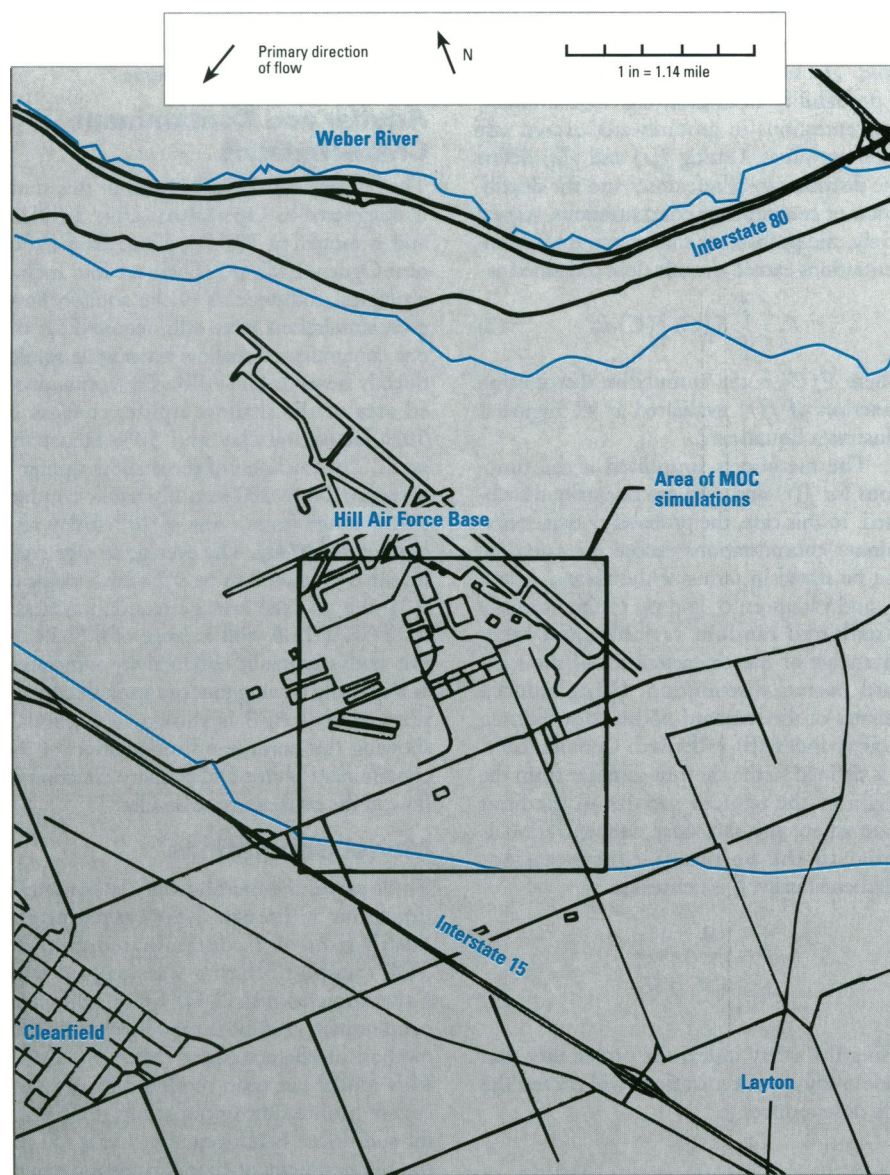
**Figure 2.** Schematic of Hill AFB, Utah. The boundaries of the boxed area designated as the area of MOC simulation represent the boundaries of the TCE contaminant plume at Hill AFB. MOC is the representation for the method of characteristics, the method used to approximate contaminant transport in this study. The groundwater flows approximately west, a direction that is perpendicular to the north–south orientation of the runway.

components of the saturated hydraulic conductivity tensor $(L\ t^{-1})$.

Equation 5 is solved to determine the spatial-time characteristics of hydraulic conductivity that are used to obtain groundwater flow velocities using Darcy's law. Darcy's law describes groundwater flow through the porous structure of the subsurface, and the 2-D version is given as

$$V_x = K_{xx}\frac{\partial h}{\partial x};\ \text{and,}\ V_y = K_{yy}\frac{\partial h}{\partial y} \tag{6}$$

where $V_x$ and $V_y$ represent the $x$ and $y$ components of the velocity vector when the

principal axes of the aquifer are aligned with those of the model. The velocity fields are then used to solve the contaminant transport model. The 2-D contaminant transport equation for a saturated porous media is given as

$$\frac{\partial}{\partial t}(C+\frac{\rho_B}{\theta}S) = \frac{\partial}{\partial x}\left[D_{xx}\frac{\partial C}{\partial x}\right]$$
$$+\frac{\partial}{\partial y}\left[D_{yy}\frac{\partial C}{\partial y}\right]$$
$$-V_x\frac{\partial C}{\partial x}-V_y\frac{\partial C}{\partial y} \tag{7}$$

where $S$ is contaminant concentration sorbed to soil/solid surfaces $(L^3\ L^{-3})$, $C$ is contaminant concentration $(M\ L^{-3})$, $\rho B$ is bulk density $(M\ L^{-3})$, $\theta$ is porosity (dimensionless), and $D_{xx}$ and $D_{yy}$ are the hydrodynamic dispersion components, $(L^2\ t^{-1})$.

In the complete description of contaminant transport in the subsurface, model equations begin by including terms for transport by convection and dispersion and a term for contaminant degradation. The term for TCE degradation (*16*) has been omitted from the contaminant transport equation for the Hill AFB aquifer because the rate of contaminant dispersive flow for this aquifer is much greater than the rate of degradation. Because of this situation, degradation of TCE will have a negligible impact on changes in TCE concentrations as a function of time and location within the aquifer. In the development of contaminant transport models, it is important to emphasize that model equations for a specific aquifer must first include terms for degradation of the contaminant by chemical and biological mechanisms along with terms describing the hydrodynamics of the aquifer. If it is determined that the rate of hydrodynamic transport is much greater than the rate of contaminant degradation, degradation terms can be omitted from the contaminant transport equation. If the rates of degradation and hydrodynamic transport are of comparable magnitude, terms describing contaminant degradation must be included.

TCE is weakly sorbed to organic matter in soils and the sorption process can be approximated by a linear Freundlich isotherm, $S = K_wC$, where $K_w$ is the equilibrium sorption coefficient $(L^3\ M^{-3})$ (*17*). Without data on longitudinal and transverse dispersivities, the dispersion coefficient is approximated as a scalar constant. With these modifications, the contaminant transport equation is given as

$$R_f\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left[D_{xx}\frac{\partial C}{\partial x}\right]+\frac{\partial}{\partial y}\left[D_{yy}\frac{\partial C}{\partial y}\right]$$
$$-V_x\frac{\partial C}{\partial x}-V_y\frac{\partial C}{\partial y} \tag{8}$$

where, for equilibrium sorption, the dimensionless retardation factor, $R_f$ is defined as

$$R_f = 1+\frac{\rho_B K_w}{\theta} \tag{9}$$

For the contaminated aquifer in this example, the distribution function for safe doses of TCE will be represented as a nor-

mal distribution with a mean of 70 µg/l, the WHO 14-day short-term exposure standard (*3*), and a standard deviation of 20 µg/l. The variance was selected arbitrarily. The bell-shaped normal distribution function using this mean and variance has a high peak with narrow width and deeply descending sides on either side of the mean. The EPA life-time exposure standard of 5 µg/l could have been chosen, but the main purpose of this study is to demonstrate how the health risks of a contaminated aquifer can be estimated. From genetic studies, there is support for representing safe doses by a normal distribution (*18*), but with the second moment method, other types of distributions can be easily accommodated.

A 38 × 39 node grid was superimposed on the area of contamination within the aquifer. The distance between nodes was 250 feet in either direction. Input data on hydrogeological and contaminant concentration characteristics were obtained from engineering reports by JMM Consulting Engineers, Inc. (*19*). Permeability testing, soil boring, a geological survey, and groundwater sampling and analyses were used to determine groundwater flow and contaminant transport behavior for the contaminated aquifer.

In this study, the hydraulic conductivity was modeled as a random variable described by a normal distribution function. The initial distribution function for the hydraulic conductivity was determined from hydrodynamic data from the contaminated aquifer. This initial distribution function was altered (optimized) using Bayesian updating to obtain a distribution function that best approximated transport behavior for this particular aquifer (*12,14,15,19*). With this updated distribution function, 100 realizations of the hydraulic conductivity field were generated using a Sequential Gaussian Simulation (SGSIM) routine from the Geostatistical Software Library (*20*). The 100 realizations of the hydraulic conductivity were entered sequentially into the contaminant transport model producing histograms of contaminant concentration at each node point. Contours of the mean contaminant concentration are shown in Figure 3. Similarly, contours depicting the probability of exceeding the safe dose concentration (*P_f*) that were generated using the second moment method given by Equation 4 are shown in Figure 4. These contour plots include the main flow direction of the aquifer and show the decrease in pollutant concentration and risk (*P_f*) as the distance from the waste site increases.

## Discussion

The second moment method presents a different approach to assessing the health risk
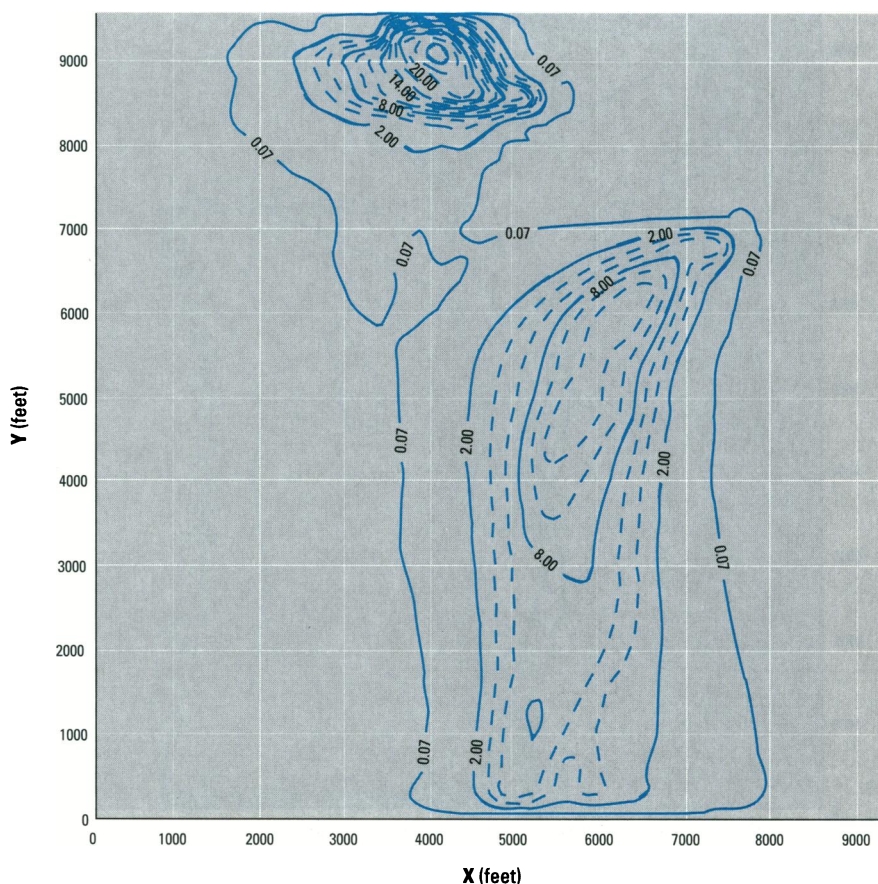


**Figure 3.** Mean concentration contours for TCE at Hill AFB (µg/l). The area of MOC simulation, the boxed area shown in Figure 2, is 9500 × 9500 feet. The contaminant plume shows two peaks, one at the top middle of this area of simulation with a maximum contaminant concentration of 26 µg/l and one to the right of the middle of the area of simulation with a maximum of 12 µg/l. The shape of the contour indicates that it is spreading in a direction that corresponds to the westerly direction of groundwater flow.

posed by a contaminant plume. Hydraulic conductivity is modeled as a normally distributed random variable. The initial distribution function for the hydraulic conductivity is optimized to approximate the transport characteristics of the aquifer. The optimized distribution is used in the contaminant transport model to produce a contaminant distribution with known mean and variance for each location within the contaminated aquifer. Safe dose concentrations have been modeled as a normal distribution with known mean and variance. These two distributions are integrated, using the second moment method, to estimate the probability of exceeding the safe dose at any location within the boundaries of the study area. In this manner, the variability of hydraulic parameters affecting pollutant concentrations in groundwater and natural variability of response to pollutant exposure in a human population are incorporated into the evaluation of the health risks of the contaminated aquifer. As such, this method makes it possible for the engineer or health scientist in the field to rapidly assess the potential

magnitude of the health risk for a contaminated aquifer and to use this information in setting priorities for cleanup. For the aquifer used in this study, the probability of exceeding safe dose concentrations is very high within the contaminant plume, as shown in Figure 4. This result is obtained because the distribution function for contaminant concentration significantly overlapped the cumulative distribution function for safe doses. Although the risk dissipates rapidly towards the boundaries of the plume, the results show that the risks are not insignificant outside the plume boundaries.

In addition, the method presented in this work provides a framework to compare and evaluate the performance of different remediation strategies and could be used as an initial screening tool in aquifer cleanup planning. In this manner, remediation technologies can be evaluated and ranked as to their effectiveness in reducing contaminant concentrations below safe doses associated with prescribed disease incidence rates. By evaluating remediation performance in this manner, a sound basis is established for
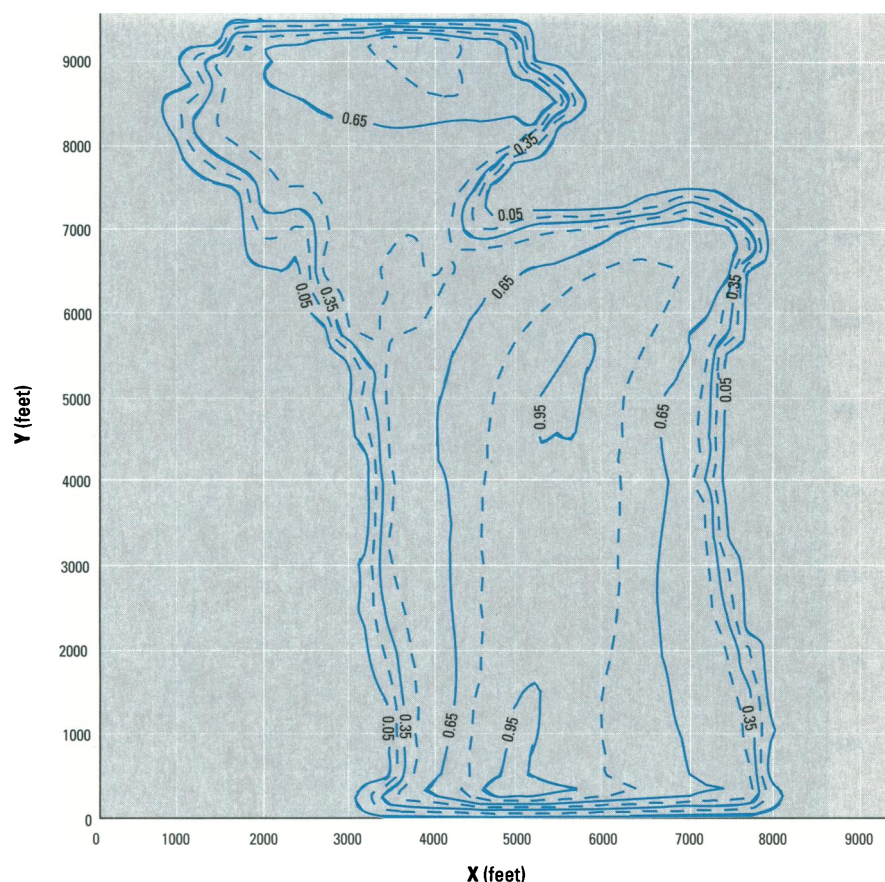
**Figure 4.** Risk contours for TCE contamination at Hill AFB. For the area of MOC simulation, the boxed area shown in Figure 2, the risk contours represent the probability of exceeding safe dose concentrations for diverse human populations. The probability is computed by Equation 2. Distributions of contaminant concentrations were computed with Equation 8 using hydrodynamic data from the contaminated aquifer. At each location in the contaminant plume, the distribution function for safe doses was normally distributed with a mean of 70 µg/l and a variance of 20 µg/l.

selecting remediation technologies that are most effective and efficient for a particular contaminant and aquifer.

A major limitation of this proposed method is the characterization of safe doses for human populations. It is not at all certain that this distribution is normal. Therefore, it could also be argued that a single deterministic safe dose would be sufficient using this method and that it is unnecessary to use a distribution of safe doses. For the aquifer used in this study, using a single safe dose or using the the EPA lifetime exposure standard of 5 µg/l would probably produce the same conclusion; however, this is an aquifer with contaminant concentrations that are several orders of magnitude greater than a single safe dose. In situations in which contaminant concentrations are close to a single safe dose exposure standard, it is not at all certain that the health risks for

a diverse human population are the same. Therefore, it is important to have a risk evaluation method that takes into account variability in exposure concentrations and safe dose levels.

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